Decision Trees

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August 13, 2025

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Introduction and Motivation

The need for interpretability

How to maintain trust in Al

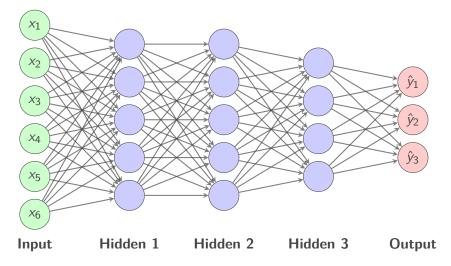
Beyond developing initial trust, however, creators of Al also must work to maintain that trust. Siau and Wang suggest seven ways of "developing continuous trust" beyond the initial phases of product development:

- Usability and reliability. At "should be designed to operate easily and intuitively,"
 Siau and Wang write. "There should be no unexpected downtime or crashes."
- Collaboration and communication. Al developers want to create systems that perform autonomously, without human involvement. Developers must focus on creating Al applications that smoothly and easily collaborate and communicate with humans.
- Sociability and bonding. Building social activities into AI applications is one way to strengthen trust. A robotic dog that can recognize its owner and show affection is one example, Siau and Wang write.
- Security and privacy protection. Al applications rely on large data sets, so
 ensuring privacy and security will be crucial to establishing trust in the
 applications.
- Interpretability. Just as transparency is instrumental in building initial trust, interpretability – or the ability for a machine to explain its conclusions or actions – will help sustain trust.

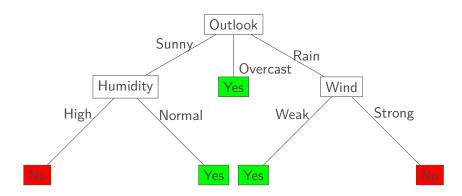
Training Data

Day	Outlook	Temp	Humidity	Windy	Play
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
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D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
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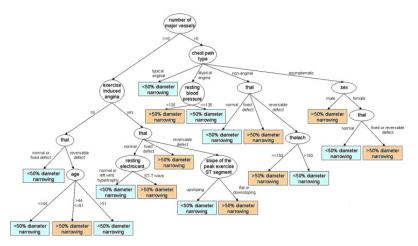
Learning a Complicated Neural Network



Learnt Decision Tree



Medical Diagnosis using Decision Trees



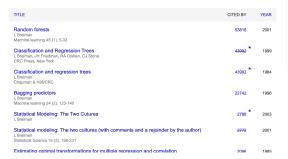
Source: Improving medical decision trees by combining relevant health-care criteria

Leo Breiman (1928-2005)



Leo Breiman 1928-2005

Professor of Statistics, <u>UC Berkeley</u>
Verified email at stat.berkeley.edu - <u>Homepage</u>
Data Analysis Statistics Machine Learning





M FOLLOW

Key Points

Major Algorithmic Breakthroughs:

• CART (1984): Classification and Regression Trees

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- Two Cultures (2001): Data Modeling vs. Algorithmic Modeling

Definition: Key Complexity Classes • P: Problems solvable in polynomial time

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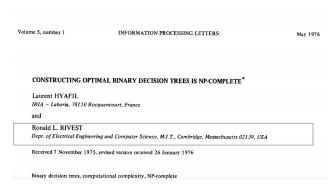
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 - Example: Optimization versions of NP-Complete problems

Finding the Optimal Decision Tree



The Problem: Given training data, find the decision tree with the highest accuracy

Important: Computational Complexity

Finding optimal decision tree is NP-Complete

- **Verification**: Given a tree, check its accuracy quickly \checkmark

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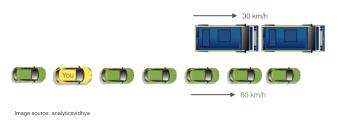
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Example: What This Means

- No efficient algorithm exists (unless P = NP)
- · Must use heuristics like greedy algorithms
- ID3, C4.5, CART use greedy approaches
- · Good solutions, but no optimality guarantee

Greedy Algorithm

Core idea: At each level, choose an attribute that gives **biggest estimated** performance gain!



 $\mathsf{Greedy} \neq \mathsf{Optimal}$

Discrete Input, Discrete Output

Day	Outlook	Temp	Humidity	Windy	Play
D1 D2 D3 D4 D5 D6 D7 D8 D9 D10 D11 D12	Sunny Sunny Overcast Rain Rain Overcast Sunny Sunny Rain Sunny Overcast	Hot Hot Hot Ocol Cool Cool Mild Cool Mild Mild Mild	High High High Normal Normal Normal Normal High Normal High	Weak Strong Weak Weak Strong Strong Weak Weak Weak Strong Strong	No No Yes Yes No Yes No Yes Yes Yes Yes
D13 D14	Overcast Rain	Hot Mild	Normal High	Weak Strong	Yes No

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For examples, we have 9 Yes,
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- Would it be trivial if we had 14 Yes or 14 No?

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- Key insight: Problem is "easier" when there is less disagreement

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- Need some statistical measure of "disagreement"

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The second one! Because it's unexpected.

Shannon's insight: The amount of information in an event should be inversely proportional to its probability.

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Why base 2? So information is measured in bits.

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• Probability: p = 0.0001 (extremely rare!)

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Notice: Rare events carry $\sim 90 \times$ more information!

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Solution: Take the **expected** (average) information!



Definition: Entropy Formula

$$H(X) = \mathbb{E}[I(X)] = -\sum_{i} p(x_i) \log_2 p(x_i)$$

 $\textbf{Entropy} = \mathsf{Expected} \ \mathsf{amount} \ \mathsf{of} \ \mathsf{information} \ \mathsf{per} \ \mathsf{observation}$

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$$H = -p(\text{rain}) \log_2 p(\text{rain}) - p(\text{cloudy}) \log_2 p(\text{cloudy})$$
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Entropy: Expected Information

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Delhi weather calculation:

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Key insight: Entropy ranges from 0 (certain) to $log_2(n)$ (uniform over n outcomes)

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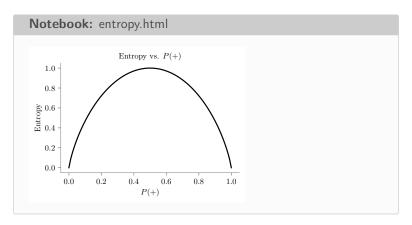
Strategy: Choose splits that **reduce entropy** the most! This is exactly what **Information Gain** measures.

Entropy

Statistical measure to characterize the (im)purity of examples

Entropy

Statistical measure to characterize the (im)purity of examples $H(X) = -\sum_{i=1}^{k} p(x_i) \log_2 p(x_i)$



Day	Outlook	Temp	Humidity	Windy	Play	Can we use Outlook as the
D1	Sunny	Hot	High	Weak	No	root node?
D2	Sunny	Hot	High	Strong	No	
D3	Overcast	Hot	High	Weak	Yes	
D4	Rain	Mild	High	Weak	Yes	
D5	Rain	Cool	Normal	Weak	Yes	
D6	Rain	Cool	Normal	Strong	No	
D7	Overcast	Cool	Normal	Strong	Yes	
D8	Sunny	Mild	High	Weak	No	
D9	Sunny	Cool	Normal	Weak	Yes	
D10	Rain	Mild	Normal	Weak	Yes	
D11	Sunny	Mild	Normal	Strong	Yes	
D12	Overcast	Mild	High	Strong	Yes	
D13	Overcast	Hot	Normal	Weak	Yes	
D14	Rain	Mild	High	Strong	No	

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D2	Sunny	Hot	High	Strong	No .
D3	Overcast	Hot	High	Weak	Yes
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D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No
	· ·	· ·	·	·	

- Can we use Outlook as the root node?
- When Outlook is overcast, we always Play and thus no "disagreement"

Information Gain

Reduction in entropy by partitioning examples (S) on attribute A

$$Gain(S, A) \equiv Entropy(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} Entropy(S_v)$$

Pop Quiz #1

Answer this!

What does entropy measure in the context of decision trees?

- A) The depth of the tree
- B) The impurity or "disagreement" in a set of examples
- C) The number of features in the dataset
- D) The accuracy of the tree

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- B) The impurity or "disagreement" in a set of examples
- C) The number of features in the dataset
- D) The accuracy of the tree

Answer: B) The impurity or "disagreement" in a set of examples — Higher entropy means more mixed classes, lower entropy means more pure subsets.

Create a root node for tree

- · Create a root node for tree
- If all examples are +/-, return root with label =+/-

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- Begin
 - $A \leftarrow$ attribute from Attributes which best classifies Examples
 - \circ Root \leftarrow A

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 - Add new tree branch : A = v

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 - For each value (v) of A
 - Add new tree branch : A = v
 - Examples_v: subset of examples that A = v
 - If Examples_vis empty: add leaf with label = most common value of Target Attribute

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- Begin
 - \circ A \leftarrow attribute from Attributes which best classifies Examples
 - \circ Root \leftarrow A
 - For each value (v) of A
 - Add new tree branch : A = v
 - Examples_v: subset of examples that A = v
 - If Examples_vis empty: add leaf with label = most common value of Target Attribute
 - Else: ID3 (Examples, Target attribute, Attributes A)

Training Data

Day	Outlook	Temp	Humidity	Windy	Play
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Entropy calculated

We have 14 examples in S: 5 No, 9 Yes

Entropy(S) =
$$-p_{No} \log_2 p_{No} - p_{Yes} \log_2 p_{Yes}$$

= $-\frac{5}{14} \log_2 \left(\frac{5}{14}\right) - \frac{9}{14} \log_2 \left(\frac{9}{14}\right) = 0.940$

Outlook	Play
Sunny	No
Sunny	No
Overcast	Yes
Rain	Yes
Rain	Yes
Rain	No
Overcast	Yes
Sunny	No
Sunny	Yes
Rain	Yes
Sunny	Yes
Overcast	Yes
Overcast	Yes
Rain	No

Outlook	Play
Sunny	No
Sunny	No
Sunny	No
Sunny	Yes
Sunny	Yes
We have 2	Yes, 3
No Entro	
$-\frac{3}{5}\log_2\left(\right.$	$(\frac{3}{5})$ -
$\frac{2}{5}\log_2\left(\frac{2}{5}\right) =$	= 0.971

Outlook | Dlaw

Outlook	Play	
Sunny	No	
Sunny	No	
Sunny	No	
Sunny	Yes	
Sunny	Yes	
We have 2	Yes, 3	
No Entro	ру =	
$-\frac{3}{5}\log_2\left(\right.$	$\left(\frac{3}{5}\right)$ –	
$\frac{2}{5}\log_2\left(\frac{2}{5}\right) =$	= 0.971	

Outlook	Play			
Overcast	Yes			
We have 4 Yes, 0				
No Entropy $= 0$				
(pure subset)				

Outlook	Play	
Sunny	No	
Sunny	No	
Sunny	No	
Sunny	Yes	
Sunny	Yes	
We have 2	Yes, 3	
No Entro	py =	
$-\frac{3}{5}\log_2\left(\right.$		
$\frac{2}{5}\log_2\left(\frac{2}{5}\right) =$	= 0.971	

Outlook	Play
Overcast	Yes
We have 4	Yes, 0
No Entrop	y = 0
(pure sul	oset)
Overcast Overcast We have 4 No Entrop	Yes Yes Yes, 0 y = 0

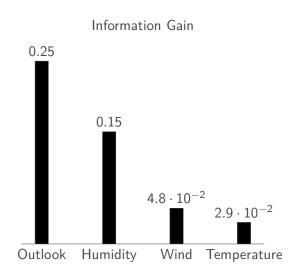
Outlook	Play
Rain	Yes
Rain	Yes
Rain	No
Rain	Yes
Rain	No
We have 3	Yes, 2
No Entro	ру =
$-\frac{3}{5}\log_2\left(\right.$	$\left(\frac{3}{5}\right)$ –
$\frac{2}{5}\log_2\left(\frac{2}{5}\right) =$	= 0.971

$$\begin{aligned} \mathsf{Gain}(S, \mathsf{Outlook}) &= \mathsf{Entropy}(S) - \\ &\sum_{v \in \{\mathsf{Rain}, \; \mathsf{Sunny}, \; \mathsf{Overcast}\}} \frac{|S_v|}{|S|} \, \mathsf{Entropy}(S_v) \end{aligned}$$

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Learnt Decision Tree



Calling ID3 on Outlook=Sunny

Day	Temp	Humidity	Windy	Play
D1	Hot	High	Weak	No
D2	Hot	High	Strong	No
D8	Mild	High	Weak	No
D9	Cool	Normal	Weak	Yes
D11	Mild	Normal	Strong	Yes

• Gain($S_{\text{Outlook}=\text{Sunny}}$, Temp) = Entropy(2 Yes, 3 No) - (2/5)*Entropy(0 Yes, 2 No) -(2/5)*Entropy(1 Yes, 1 No) - (1/5)*Entropy(1 Yes, 0 No)

Calling ID3 on Outlook=Sunny

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D11	Mild	Normal	Strong	Yes

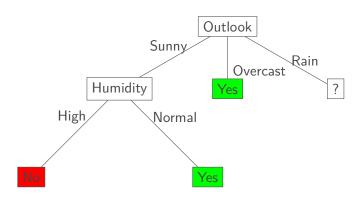
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- Gain(S_{Outlook=Sunny}, Humidity) = Entropy(2 Yes, 3 No) (2/5)*Entropy(2 Yes, 0 No) -(3/5)*Entropy(0 Yes, 3 No) ⇒ maximum possible for the set

Calling ID3 on Outlook=Sunny

Day	Temp	Humidity	Windy	Play
D1	Hot	High	Weak	No
D2	Hot	High	Strong	No
D8	Mild	High	Weak	No
D9	Cool	Normal	Weak	Yes
D11	Mild	Normal	Strong	Yes

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- Gain(S_{Outlook=Sunny}, Humidity) = Entropy(2 Yes, 3 No) (2/5)*Entropy(2 Yes, 0 No) -(3/5)*Entropy(0 Yes, 3 No) ⇒ maximum possible for the set
- $Gain(S_{Outlook=Sunny}, Windy) = Entropy(2 Yes, 3 No) (3/5)*Entropy(1 Yes, 2 No) (2/5)*Entropy(1 Yes, 1 No)$

Learnt Decision Tree

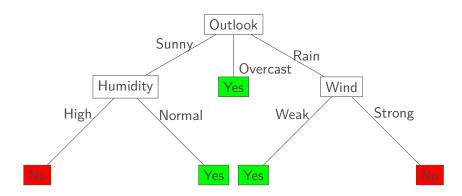


Calling ID3 on (Outlook=Rain)

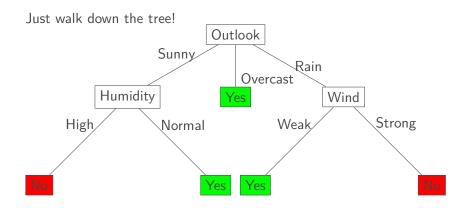
Day	Temp	Humidity	Windy	Play
D4	Mild	High	Weak	Yes
D5	Cool	Normal	Weak	Yes
D6	Cool	Normal	Strong	No
D10	Mild	Normal	Weak	Yes
D14	Mild	High	Strong	No

• The attribute Windy gives the highest information gain

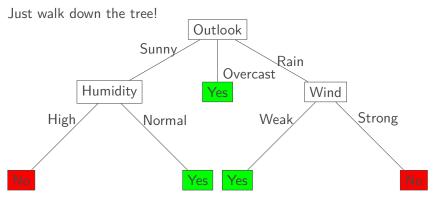
Learnt Decision Tree



Prediction for Decision Tree

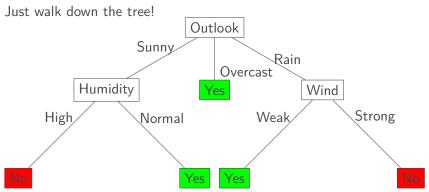


Prediction for Decision Tree



Prediction for <High Humidity, Strong Wind, Sunny Outlook, Hot Temp> is ?

Prediction for Decision Tree



Prediction for <High Humidity, Strong Wind, Sunny Outlook, Hot Temp> is ? No

Definition: Depth-Limited Trees

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When depth limit is reached, assign the **most common class** in that path as the leaf node prediction.

Depth-0 tree (no decisions):

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Pop Quiz #3

Answer this!

In the tennis dataset, why did "Outlook" have the highest information gain?

- A) It was the first feature in the dataset
- B) When Outlook=Overcast, all examples have Play=Yes (pure subset)
- C) It has the most possible values
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Answer: B) When Outlook=Overcast, all examples have Play=Yes - This creates a pure subset with entropy=0, maximizing information gain.

Discrete Input, Real Output

Modified Dataset

Day	Outlook	Temp	Humidity	Wind	Minutes Played
D1	Sunny	Hot	High	Weak	20
D2	Sunny	Hot	High	Strong	24
D3	Overcast	Hot	High	Weak	40
D4	Rain	Mild	High	Weak	50
D5	Rain	Cool	Normal	Weak	60
D6	Rain	Cool	Normal	Strong	10
D7	Overcast	Cool	Normal	Strong	4
D8	Sunny	Mild	High	Weak	10
D9	Sunny	Cool	Normal	Weak	60
D10	Rain	Mild	Normal	Weak	40
D11	Sunny	Mild	High	Strong	45
D12	Overcast	Mild	High	Strong	40
D13	Overcast	Hot	Normal	Weak	35
D14	Rain	Mild	High	Strong	20

Classification trees predict discrete classes (Yes/No, categories)

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- For regression: Use Mean Squared Error (MSE)

Key Points

Why MSE for Regression?

MSE measures how far predicted values are from actual values.

Lower $\mathsf{MSE} = \mathsf{Better}\ \mathsf{predictions} = \mathsf{Less}\ \mathsf{``impurity''}\ \mathsf{in}\ \mathsf{the}$ data

Definition: Mean Squared Error

For a dataset S with n data points and target values y_1, y_2, \dots, y_n :

$$MSE(S) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \bar{y})^2$$

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where $\bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$ is the mean of target values

• $(y_i - \bar{y})^2$: Squared difference between actual and mean

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- MSE = 0 when all values are identical (perfect homogeneity)
- Higher MSE = More variation = Higher impurity

MSE Calculation: Step 1 - The Complete Dataset

Wind	Minutes Played
Weak	20
Strong	24
Weak	40
Weak	50
Weak	60
Strong	10
Strong	4
Weak	10
Weak	60
Weak	40
Strong	45
Strong	40
Weak	35
Strong	20

• Tennis Dataset: Predicting minutes played (continuous target)

MSE Calculation: Step 1 - The Complete Dataset

Wind	Minutes Played
Weak	20
Strong	24
Weak	40
Weak	50
Weak	60
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Strong	4
Weak	10
Weak	60
Weak	40
Strong	45
Strong	40
Weak	35
Strong	20

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- Goal: Calculate MSE for the entire dataset S

MSE Calculation: Step 1 - The Complete Dataset

Wind	Minutes Played
Weak	20
Strong	24
Weak	40
Weak	50
Weak	60
Strong	10
Strong	4
Weak	10
Weak	60
Weak	40
Strong	45
Strong	40
Weak	35
Strong	20

- Tennis Dataset: Predicting minutes played (continuous target)
- Goal: Calculate MSE for the entire dataset S
- Step 1: Find the mean \bar{y} of all target values

Example: Calculating Mean Minutes Played

All target values: 20, 24, 40, 50, 60, 10, 4, 10, 60, 40, 45, 40, 35, 20

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Step 1: Sum all values

$$\sum y_i = 20 + 24 + 40 + 50 + 60 + 10 + 4 + 10$$
$$+ 60 + 40 + 45 + 40 + 35 + 20$$

Example: Calculating Mean Minutes Played

All target values: 20, 24, 40, 50, 60, 10, 4, 10, 60, 40, 45, 40, 35, 20

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$$\sum y_i = 20 + 24 + 40 + 50 + 60 + 10 + 4 + 10$$
$$+ 60 + 40 + 45 + 40 + 35 + 20$$
$$= 458$$

Example: Calculating Mean Minutes Played

All target values: 20, 24, 40, 50, 60, 10, 4, 10, 60, 40, 45, 40, 35, 20

Step 1: Sum all values

$$\sum y_i = 20 + 24 + 40 + 50 + 60 + 10 + 4 + 10$$
$$+ 60 + 40 + 45 + 40 + 35 + 20$$
$$= 458$$

Step 2: Divide by number of data points (n = 14)

$$\bar{y} = \frac{458}{14} = 32.71$$
 minutes

MSE Calculation: Step 3 - Computing Squared Differences

Example: Calculating $(y_i - \bar{y})^2$ for Each Data Point

With $\bar{y} = 32.71$:

Уi	$y_i - \bar{y}$	$(y_i - \bar{y})^2$
20	20 - 32.71 = -12.71	$(-12.71)^2 = 161.54$
24	24 - 32.71 = -8.71	$(-8.71)^2 = 75.86$
40	40 - 32.71 = 7.29	$(7.29)^2 = 53.14$
50	50 - 32.71 = 17.29	$(17.29)^2 = 299.14$
60	60 - 32.71 = 27.29	$(27.29)^2 = 744.74$
10	10 - 32.71 = -22.71	$(-22.71)^2 = 515.74$
4	4 - 32.71 = -28.71	$(-28.71)^2 = 824.26$

MSE Calculation: Step 3 - Computing Squared Differences

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10	10 - 32.71 = -22.71	$(-22.71)^2 = 515.74$
4	4 - 32.71 = -28.71	$(-28.71)^2 = 824.26$

Continue this for all 14 data points...

MSE Calculation: Step 4 - Complete Squared Differences

Example: All Squared Differences

Уi	$y_i - \bar{y}$	$(y_i - \bar{y})^2$
20	-12.71	161.54
24	-8.71	75.86
40	7.29	53.14
50	17.29	299.14
60	27.29	744.74
10	-22.71	515.74
4	-28.71	824.26
10	-22.71	515.74
60	27.29	744.74
40	7.29	53.14
45	12.29	151.04
40	7.29	53.14
35	2.29	5.24
20	-12.71	161.54
Sum		4358.86

Example: Computing MSE for Complete Dataset

Formula:

$$MSE(S) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \bar{y})^2$$

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Substituting our values:

$$\mathsf{MSE}(S) = \frac{1}{14} \times 4358.86 = 311.35$$

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Interpretation:

• MSE = 311.35 square-minutes

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Interpretation:

- MSE = 311.35 square-minutes
- · This measures the "impurity" or variation in our dataset

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$$MSE(S) = \frac{1}{14} \times 4358.86 = 311.35$$

Interpretation:

- MSE = 311.35 square-minutes
- · This measures the "impurity" or variation in our dataset
- Higher MSE = More variation in target values

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Interpretation:

- MSE = 311.35 square-minutes
- This measures the "impurity" or variation in our dataset
- Higher MSE = More variation in target values
- · When we split the data, we want to reduce this MSE

Definition: MSE Reduction Formula

For a split on attribute A with values v_1, v_2, \ldots, v_k :

$$\mathsf{MSE} \; \mathsf{Reduction} = \mathsf{MSE}(S) - \sum_{j=1}^k \frac{|S_{v_j}|}{|S|} \times \mathsf{MSE}(S_{v_j})$$

where:

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- |S| is the size of original dataset

Definition: MSE Reduction Formula

For a split on attribute A with values v_1, v_2, \ldots, v_k :

$$\mathsf{MSE}\ \mathsf{Reduction} = \mathsf{MSE}(S) - \sum_{j=1}^{\kappa} \frac{|S_{v_j}|}{|S|} \times \mathsf{MSE}(S_{v_j})$$

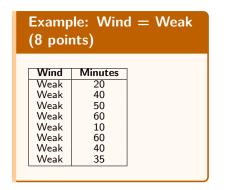
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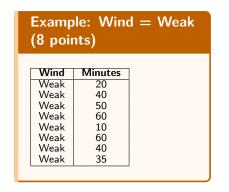
Key Points

Key Insight: MSE Reduction > 0 means the split improves our model! **Choose the split with highest MSE Reduction**

	Example: Wind = Weak (8 points)		
Wind	Minutes]	
Weak	20		
Weak	40		
Weak	50		
Weak	60		
Weak	10		
Weak	60		
Weak	40		
Weak	35		

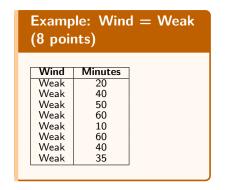






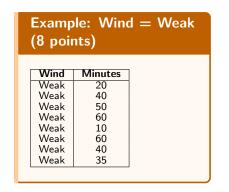
	Example: Wind = Strong (6 points)		
Wind	Minutes	1	
Strong	24	1	
Strong	10		
Strong	4		
Strong	45		
Strong	40		
Strong	20		

• Original dataset: 14 points, MSE = 311.35



Example: Wind = Strong (6 points)		
Minutes]	
24	1	
10		
4		
45		
40		
20		
<u> </u>		
	Minutes 24 10 4 45 40	Minutes 24 10 4 45 40

- Original dataset: 14 points, MSE = 311.35
- **After split:** 8 points (Weak) + 6 points (Strong)



	Example: Wind = Strong (6 points)		
Wind	Minutes]	
Strong	24	1	
Strong	10		
Strong	4		
Strong	45		
Strong	40		
Strong	20		
<u> </u>			

- Original dataset: 14 points, MSE = 311.35
- **After split:** 8 points (Weak) + 6 points (Strong)
- Next: Calculate MSE for each subset

Splitting on Wind: Step 2 - MSE for Wind=Weak

Example: Calculating $MSE(S_{Wind=Weak})$

Data points: 20, 40, 50, 60, 10, 60, 40, 35

Splitting on Wind: Step 2 - MSE for Wind=Weak

Example: Calculating $MSE(S_{Wind=Weak})$

Data points: 20, 40, 50, 60, 10, 60, 40, 35

Step 1: Calculate mean

$$ar{y}_{\text{weak}} = rac{20 + 40 + 50 + 60 + 10 + 60 + 40 + 35}{8}$$
 $= rac{315}{8} = 39.375$

Splitting on Wind: Step 2 - MSE for Wind=Weak

Example: Calculating $MSE(S_{Wind=Weak})$

Data points: 20, 40, 50, 60, 10, 60, 40, 35

Step 1: Calculate mean

$$ar{y}_{\text{weak}} = rac{20 + 40 + 50 + 60 + 10 + 60 + 40 + 35}{8}$$

$$= rac{315}{8} = 39.375$$

Step		2:	Calculate
	Уi	$y_i - 39.375$	$(y_i - 39.375)^2$
	20	-19.375	375.39
	40	0.625	0.39
	50	10.625	112.89
	60	20.625	425.39
	10	-29.375	862.89
	60	20.625	425.39
	40	0.625	0.39
	35	-4.375	19.14
	Sum		2221 87

squared differences

Splitting on Wind: Step 3 - Complete MSE for Wind=Weak

Example: Final MSE Calculation for Wind=Weak

$$MSE(S_{Wind=Weak}) = \frac{1}{8} \times 2221.87 = 277.73$$

Example: Final MSE Calculation for Wind=Weak

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Example: Verification Check

• Original MSE for all data: 311.35

Example: Final MSE Calculation for Wind=Weak

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- Original MSE for all data: 311.35
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Example: Final MSE Calculation for Wind=Weak

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Example: Verification Check

- Original MSE for all data: 311.35
- MSE for Wind=Weak subset: 277.73
- Good sign: MSE decreased (less variation within this group)

Example: Final MSE Calculation for Wind=Weak

$$MSE(S_{Wind=Weak}) = \frac{1}{8} \times 2221.87 = 277.73$$

Example: Verification Check

- Original MSE for all data: 311.35
- MSE for Wind=Weak subset: 277.73
- Good sign: MSE decreased (less variation within this group)
- This subset is more "homogeneous" than the full dataset

Example: Calculating $MSE(S_{Wind=Strong})$

Data points: 24, 10, 4, 45, 40, 20

Example: Calculating $MSE(S_{Wind=Strong})$

Data points: 24, 10, 4, 45, 40, 20

Step 1: Calculate mean

$$\bar{y}_{\text{strong}} = \frac{24 + 10 + 4 + 45 + 40 + 20}{6} = \frac{143}{6} = 23.83$$

Example: Calculating $MSE(S_{Wind=Strong})$

Data points: 24, 10, 4, 45, 40, 20

Step 1: Calculate mean

$$\bar{y}_{\text{strong}} = \frac{24 + 10 + 4 + 45 + 40 + 20}{6} = \frac{143}{6} = 23.83$$

Step 2: Calculate squared differences

	Уi	$y_i - 23.83$	$(y_i - 23.83)^2$	
ſ	24	0.17	0.03	
	10	-13.83	191.27	
ı	4	-19.83	393.23	
	45	21.17	448.17	
ı	40	16.17	261.47	
١	20 -3.83		14.67	
Ì	Sum		1308.84	

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Sum		1308.84

$$\mathsf{MSE}(S_{\mathsf{Wind}=\mathsf{Strong}}) = \frac{1}{6} \times 1308.84 = 218.14$$

Example: Final MSE Reduction Calculation

We have:

• MSE(S) = 311.35 (original dataset)

Example: Final MSE Reduction Calculation

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Example: Final MSE Reduction Calculation

We have:

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- $MSE(S_{Wind=Weak}) = 277.73$ (8 points)
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Weighted Average MSE:

Weighted MSE =
$$\frac{8}{14} \times 277.73 + \frac{6}{14} \times 218.14$$

= $0.571 \times 277.73 + 0.429 \times 218.14$
= $158.60 + 93.58 = 252.18$

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= $0.571 \times 277.73 + 0.429 \times 218.14$
= $158.60 + 93.58 = 252.18$

MSE Reduction:

MSE Reduction =
$$311.35 - 252.18 = 59.17$$

Key Points

What Does MSE Reduction = 59.17 Mean?

• Positive value: The split improves our model!

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- Intuition: Wind attribute helps separate high/low playing minutes

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Example: Decision Tree Building Process

• Step 1: Calculate MSE reduction for all possible splits

Key Points

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- **Step 1**: Calculate MSE reduction for all possible splits
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- Stop when: MSE reduction becomes too small or max depth reached

Important: Key Difference from Classification

Classification: Use Information Gain (maximize information) **Regression:** Use MSE Reduction (minimize prediction error)

Pop Quiz #5

Answer this!

For regression trees, what criterion do we use instead of Information Gain?

- A) Information Gain
- B) Gini Impurity
- C) Mean Squared Error (MSE) Reduction
- D) Accuracy

Pop Quiz #5

Answer this!

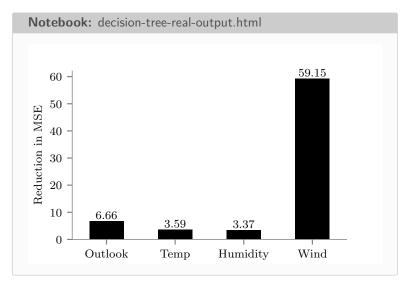
For regression trees, what criterion do we use instead of Information Gain?

- A) Information Gain
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- C) Mean Squared Error (MSE) Reduction
- D) Accuracy

Answer: C) Mean Squared Error (MSE) Reduction

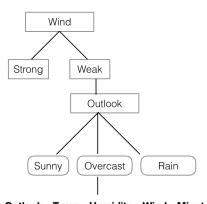
- For regression, we minimize MSE instead of maximizing information gain.

MSE Reduction for Regression Trees



Learnt Tree

Assume a tree like this is learnt ...



		Day	Outlook	Temp	Humidity	Wind	Minutes Played
	2	D3	Overcast	Hot	High	Weak	40
	12	D13	Overcast	Hot	Normal	Weak	35

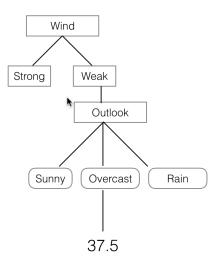
Learnt Tree

Method 1

Mins

Played=(40+35)

/2



Real Input, Discrete Output

Key Points

Our Journey Through Decision Tree Types:

• Discrete Input, Discrete Output: Simple categorical splits

Key Points

Our Journey Through Decision Tree Types:

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- · Real Input, Real Output: Continuous features, regression trees

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Key Points

Our Journey Through Decision Tree Types:

- · Discrete Input, Discrete Output: Simple categorical splits
- Real Input, Real Output: Continuous features, regression trees
- Real Input, Discrete Output: Continuous features, classification

What's different now?

 Input: Continuous/real-valued features (like temperature, age, income)

Key Points

Our Journey Through Decision Tree Types:

- Discrete Input, Discrete Output: Simple categorical splits
- · Real Input, Real Output: Continuous features, regression trees
- Real Input, Discrete Output: Continuous features, classification

- Input: Continuous/real-valued features (like temperature, age, income)
- Output: Discrete classes (Yes/No, Low/Medium/High, etc.)

Key Points

Our Journey Through Decision Tree Types:

- Discrete Input, Discrete Output: Simple categorical splits
- Real Input, Real Output: Continuous features, regression trees
- Real Input, Discrete Output: Continuous features, classification

- Input: Continuous/real-valued features (like temperature, age, income)
- Output: Discrete classes (Yes/No, Low/Medium/High, etc.)
- Challenge: Where exactly should we split the continuous feature?

The Key Challenge: Infinite Split Points

Important: The Problem

With continuous features, we have potentially infinite split points!

• Temperature could be split at 45°C, 45.1°C, 45.01°C, ...

The Intuitive Solution:

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- · We need a systematic approach to find the best split points

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1. Look for "natural boundaries" between different classes

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- 1. Look for "natural boundaries" between different classes
- 2. Focus on points where class labels actually change

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With continuous features, we have potentially infinite split points!

- Temperature could be split at 45°C, 45.1°C, 45.01°C, ...
- · We need a systematic approach to find the best split points

The Intuitive Solution:

- 1. Look for "natural boundaries" between different classes
- 2. Focus on points where class labels actually change
- 3. Test splits that maximize information gain

The Tennis Example - Setting the Stage

Scenario: Should we play tennis based on temperature?

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

Question: How do we find the best split point in this continuous temperature data?

Example: Why Sort the Data First?

· Sorting reveals the natural class boundaries in the data

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
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Example: Why Sort the Data First?

- · Sorting reveals the natural class boundaries in the data
- We can see where labels change: No ightarrow Yes ightarrow No

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Example: Why Sort the Data First?

- · Sorting reveals the natural class boundaries in the data
- We can see where labels change: No ightarrow Yes ightarrow No
- · Only need to consider splits between different class labels

Day	Temperature	PlayTennis
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D6	90	No

Example: Why Sort the Data First?

- · Sorting reveals the natural class boundaries in the data
- We can see where labels change: No \rightarrow Yes \rightarrow No
- Only need to consider splits between different class labels
- · Eliminates millions of irrelevant split points!

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

Definition: The Midpoint Strategy

Only consider splits at midpoints between consecutive different classes:

• Between 48(No) and 60(Yes): split at (48 + 60)/2 = 54

All candidate splits: 44, 54, 66, 76, 85

Key Points

Definition: The Midpoint Strategy

Only consider splits at midpoints between consecutive different classes:

- Between 48(No) and 60(Yes): split at (48 + 60)/2 = 54
- Between 80(Yes) and 90(No): split at (80 + 90)/2 = 85

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Key Points

Definition: The Midpoint Strategy

Only consider splits at midpoints between consecutive different classes:

- Between 48(No) and 60(Yes): split at (48 + 60)/2 = 54
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All candidate splits: 44, 54, 66, 76, 85

Key Points

Why These 5 Splits?

• 44: Separates D1 from rest

Definition: The Midpoint Strategy

Only consider splits at midpoints between consecutive different classes:

- Between 48(No) and 60(Yes): split at (48 + 60)/2 = 54
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Key Points

- 44: Separates D1 from rest
- 54: Separates No's from Yes's

Definition: The Midpoint Strategy

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- Between 48(No) and 60(Yes): split at (48 + 60)/2 = 54
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Key Points

- 44: Separates D1 from rest
- 54: Separates No's from Yes's
- 66, 76: Split within the Yes region

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Key Points

- 44: Separates D1 from rest
- 54: Separates No's from Yes's
- 66, 76: Split within the Yes region
- 85: Separates last Yes from final No

Evaluating Split at Temperature ≤ 44

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

Example: Split Analysis

Left side (Temp \leq **44):** 1 example, all "No" \rightarrow Perfect purity!

Right side (Temp > **44):** 5 examples, 3 "Yes", 2 "No" \rightarrow

Mixed

Entropy(Left) = 0, Entropy(Right) = 0.971

Weighted Entropy = $\frac{1}{6} \times 0 + \frac{5}{6} \times 0.971 = 0.808$

Evaluating Split at Temperature ≤ 54

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

Example: Split Analysis

Left side (Temp \leq **54):** 2 examples, all "No" \rightarrow Perfect purity!

Right side (Temp > 54): 4 examples, 3 "Yes", 1 "No" \rightarrow

Better!

Entropy(Left) = 0, Entropy(Right) = 0.811

Weighted Entropy = $\frac{2}{6} \times 0 + \frac{4}{6} \times 0.811 = 0.541$

Comparing All Candidate Splits

Split Point	Left Side	Right Side	Weighted Entropy	Info Gain
44 54 66 76	1 No 2 No 2 No, 1 Yes 2 No, 2 Yes	3 Yes, 2 No 3 Yes, 1 No 2 Yes, 1 No 1 Yes, 1 No	0.808 0.541 0.918 1.000	0.142 0.409 0.032 -0.050
85	2 No, 3 Yes	1 No	0.650	0.300

Key Points

Winner: Split at 54!

• Lowest weighted entropy (0.541)

Comparing All Candidate Splits

Split Point	Left Side	Right Side	Weighted Entropy	Info Gain
44	1 No	3 Yes, 2 No	0.808	0.142
54	2 No	3 Yes, 1 No	0.541	0.409
66	2 No, 1 Yes	2 Yes, 1 No	0.918	0.032
76	2 No, 2 Yes	1 Yes, 1 No	1.000	-0.050
85	2 No, 3 Yes	1 No	0.650	0.300

Key Points

Winner: Split at 54!

- Lowest weighted entropy (0.541)
- Highest information gain (0.409)

Comparing All Candidate Splits

Split Point	Left Side	Right Side	Weighted Entropy	Info Gain
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54	2 No	3 Yes, 1 No	0.541	0.409
66	2 No, 1 Yes	2 Yes, 1 No	0.918	0.032
76	2 No, 2 Yes	1 Yes, 1 No	1.000	-0.050
85	2 No, 3 Yes	1 No	0.650	0.300

Key Points

Winner: Split at 54!

- Lowest weighted entropy (0.541)
- Highest information gain (0.409)
- · Creates the best class separation

Definition: Decision Tree Algorithm for Continuous Features

1. Sort data by feature values

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- Identify candidate split points (midpoints between different classes)

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 - Information Gain = Original Entropy Weighted Entropy

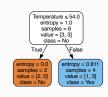
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- 3. **Evaluate** each split using information gain:
 - Calculate weighted entropy for the split
 - Information Gain = Original Entropy Weighted Entropy
- 4. Choose split with highest information gain
- 5. Recurse on left and right subsets

Visual Example: The Resulting Decision Tree

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

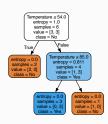
Notebook: decision-tree-real-input-discrete-output.html



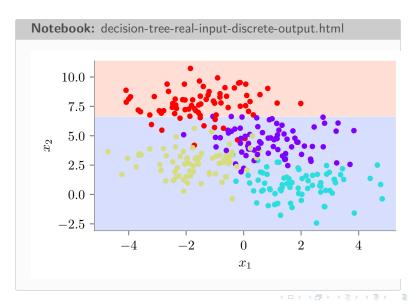
Finding splits

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D5	80	Yes
D6	90	No

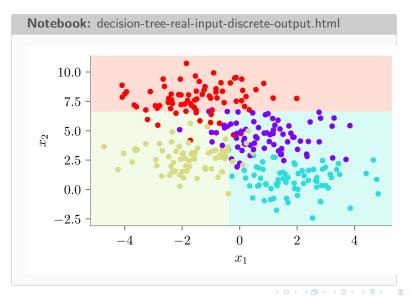
Notebook: decision-tree-real-input-discrete-output.html



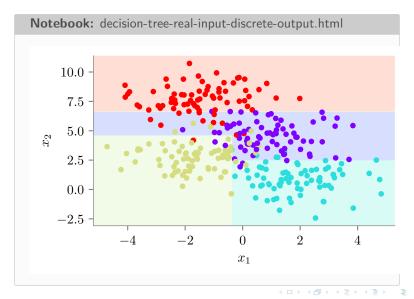
Example (DT of depth 1)



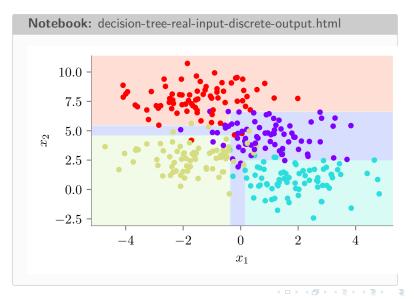
Example (DT of depth 2)



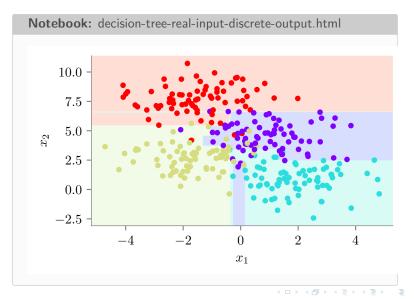
Example (DT of depth 3)



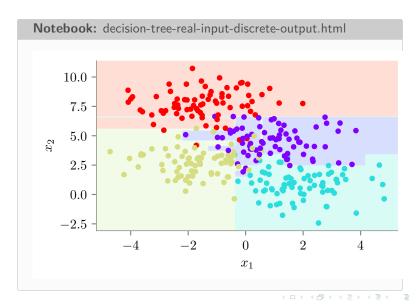
Example (DT of depth 4)



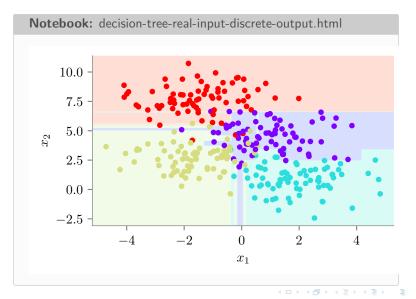
Example (DT of depth 5)



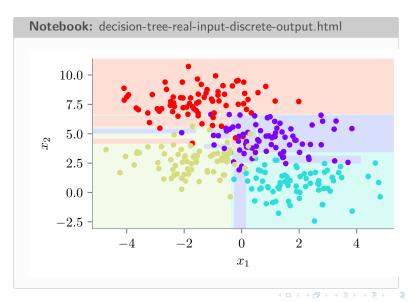
Example (DT of depth 6)



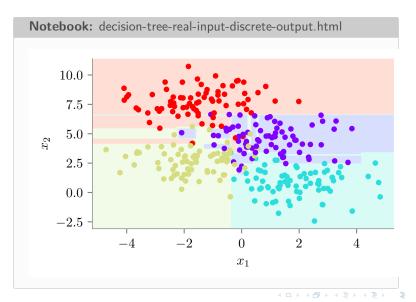
Example (DT of depth 7)



Example (DT of depth 8)



Example (DT of depth 9)



Pop Quiz #7

Answer this!

When finding splits for continuous features, how do we determine candidate split points?

- A) Use all feature values as split points
- B) Use midpoints between consecutive sorted feature values
- C) Use random values within the feature range
- D) Use only the minimum and maximum values

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Answer: B) Use midpoints between consecutive sorted feature values - This ensures we test all meaningful boundaries between different class regions.

Real Input, Real Output

Key Points

Our Decision Tree Journey - Final Stop:

• Discrete Input, Discrete Output: Categorical splits, entropy

Key Points

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What we learned:

• From Case 2: Use MSE for regression, predict means in leaves

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- Case 4: Combine both approaches for regression trees!

Example: From Case 3 (Real Input, Discrete Output)

• Sorting Strategy: Sort by feature values to find natural boundaries

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- · Weighted Loss: Consider subset sizes in evaluation

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- 2. Use Case 2's MSE-based evaluation criteria

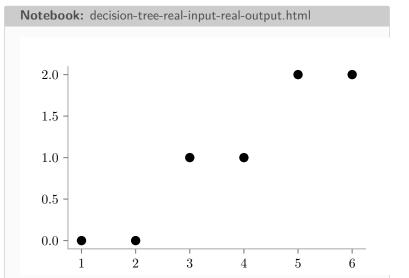
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- 3. Weight by sample sizes for fair comparison

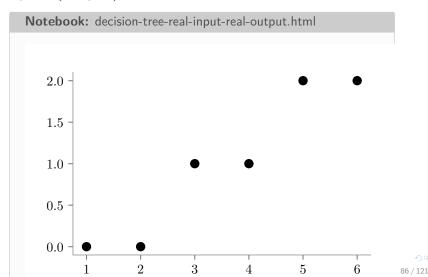
Example Dataset

Let us consider the regression dataset below:



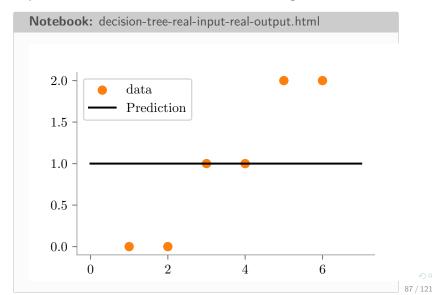
Baseline: Decision Tree with Depth 0

Question: What would be the prediction for decision tree with depth 0 (no splits)?



Baseline Performance Visualization

Depth 0 Prediction: Horizontal line = average of all Y values



Finding Split Candidates - Learning from Case 3

Definition: Split Candidate Strategy (from Case 3)

1. **Sort** data points by X values: $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$

Why midpoints? They ensure we capture all meaningful boundaries where the trend might change.

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Split candidates =
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3. Evaluate each split using MSE reduction (not entropy!)

Why midpoints? They ensure we capture all meaningful boundaries where the trend might change.

Objective Function for Regression Trees - Setup

Feature is denoted by X and target by Y.

Let the split be at X = s.

Define regions: $R_1 = \{x : x \le s\}$ and $R_2 = \{x : x > s\}$.

For each region, compute the mean prediction:

$$c_1 = \frac{1}{|R_1|} \sum_{x_i \in R_1} y_i$$
 and $c_2 = \frac{1}{|R_2|} \sum_{x_i \in R_2} y_i$

Objective Function - Weighted MSE

Example: Sample-Weighted MSE

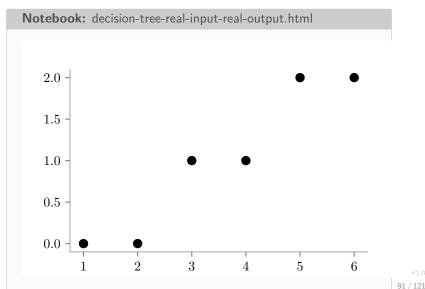
Weighted Loss(s) =
$$\frac{|R_1|}{|R_1| + |R_2|} \cdot \mathsf{MSE}(R_1) + \frac{|R_2|}{|R_1| + |R_2|} \cdot \mathsf{MSE}(R_2)$$

Where:
$$MSE(R_i) = \frac{1}{|R_i|} \sum_{x_i \in R_i} (y_j - c_i)^2$$

Our objective: $s^* = \arg\min_s \text{Weighted Loss}(s)$

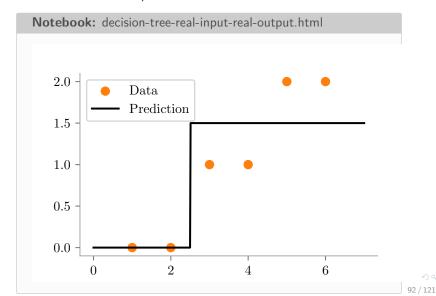
Example: Finding the Best Split

What would be the decision tree with depth 1?



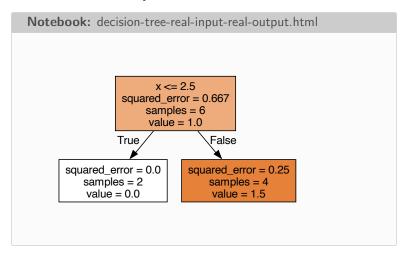
Example 1

Decision tree with depth 1



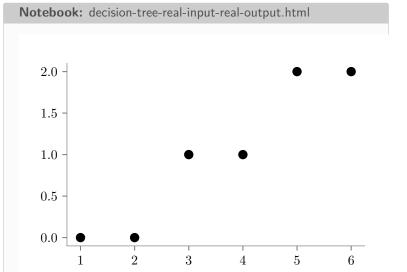
Example 1

The Decision Boundary



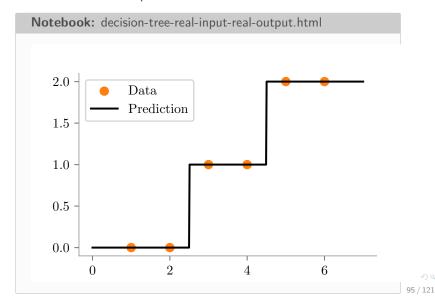
Example 1

What would be the decision tree with depth 2?



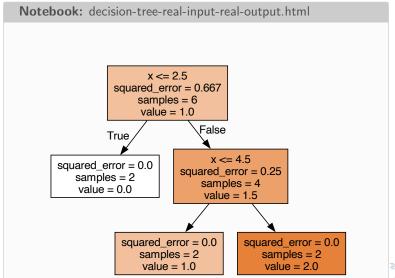
Example 1

Decision tree with depth 2



Example 1

The Decision Boundary



Algorithm: Finding the Optimal Split

1. Sort all data points (x_i, y_i) in increasing order of x_i .

Algorithm: Finding the Optimal Split

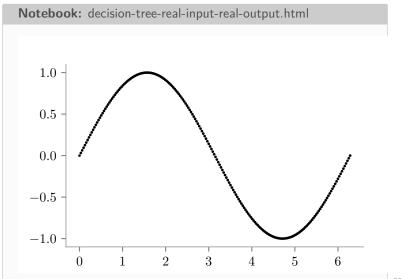
- 1. Sort all data points (x_i, y_i) in increasing order of x_i .
- 2. Evaluate the loss function for all candidate splits:

$$s = \frac{x_i + x_{i+1}}{2}$$
 for $i = 1, 2, ..., n-1$

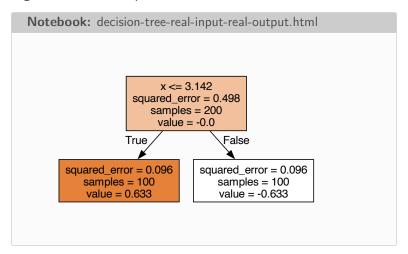
3. Select the split s^* that minimizes the loss function.

Draw a regression tree for Y = $\sin(X)$, $0 \le X \le 2\pi$

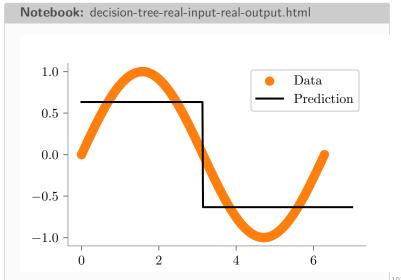
Dataset of Y = $\sin(X)$, $0 \le X \le 7$ with 10,000 points



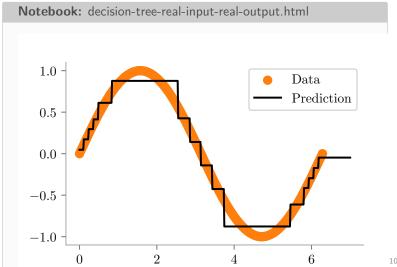
Regression tree of depth 1



Decision Boundary



Regression tree with no depth limit is too big to fit in a slide. It has of depth 4. The decision boundaries are in figure below.



Pop Quiz #8

Answer this!

What is the prediction function for a regression tree leaf node?

- A) The median of target values
- B) The mode of target values
- C) The mean of target values
- D) A linear function

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Answer: C) The mean of target values

Weighted Entropy

Key Points

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- Weighted entropy respects point importance.

Weighted Entropy Formula

For dataset S with points (x_j, y_j) and weights w_j :

$$H_w(S) = -\sum_{c \in \mathcal{C}} \underbrace{\frac{\sum_{j \in c} w_j}{\sum_{j \in S} w_j}}_{\text{Weighted } P(c)} \log_2 \left(\frac{\sum_{j \in c} w_j}{\sum_{j \in S} w_j} \right)$$

• w_j : weight of point j (can be fractional)

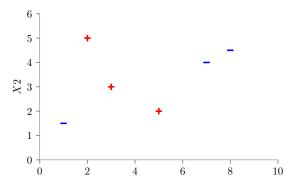
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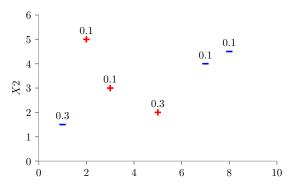
- w_j : weight of point j (can be fractional)
- C: set of classes

Weighted Entropy



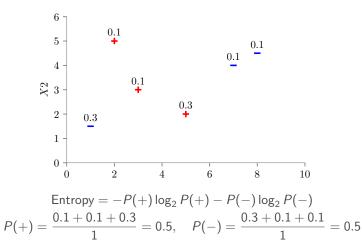
Setup: We start with mixed data - let's see how splitting helps us achieve purity

Weighted Entropy



Original Entropy Calculation:

Computing Original Entropy

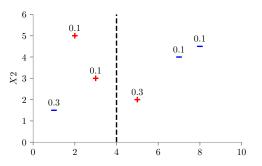


Entropy =
$$E_s = -\frac{1}{2}\log_2\frac{1}{2} - \frac{1}{2}\log_2\frac{1}{2} = 1$$

Maximum impurity! Perfect 50-50 split

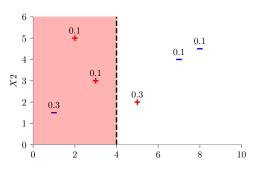


Choosing a Split



Candidate Split: $X_1 = 4$ (denoted as X_1^*) Let's see if this vertical line creates purer subsets!

Left Subset: $X_1 \leq X_1^*$



Computing entropy of left subset:

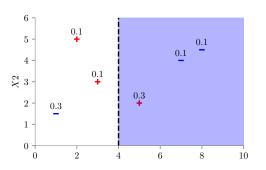
$$P(+) = \frac{0.1 + 0.1}{0.1 + 0.1 + 0.3} = \frac{2}{5} = 0.4$$

$$P(-) = \frac{0.3}{0.5} = \frac{3}{5} = 0.6$$

$$H(left) = -0.4 \log_2(0.4) - 0.6 \log_2(0.6) \approx 0.971$$

110/121

Right Subset: $X_1 > X_1^*$



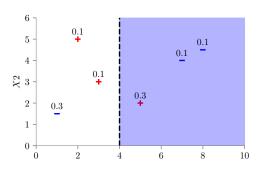
Computing entropy of right subset:

$$P(+) = \frac{0.3}{0.3 + 0.2} = \frac{3}{5} = 0.6$$

$$P(-) = \frac{0.2}{0.5} = \frac{2}{5} = 0.4$$

$$H(\text{right}) = -0.6 \log_2(0.6) - 0.4 \log_2(0.4) \approx 0.971$$

Computing Weighted Entropy



Example: Weighted Entropy Calculation

Weighted Entropy
$$= \frac{|S_{\text{left}}|}{|S|} \cdot H(\text{left}) + \frac{|S_{\text{right}}|}{|S|} \cdot H(\text{right})$$
$$= \frac{0.5}{1.0} \cdot 0.971 + \frac{0.5}{1.0} \cdot 0.971$$
$$= 0.5 \times 0.971 + 0.5 \times 0.971 = 0.971$$

Information Gain Calculation

Key Points

Information Gain = Original Entropy - Weighted Entropy

$$\mathsf{IG}(X_1 = X_1^*) = E_S - \mathsf{Weighted}$$
 Entropy

$$= 1.0 - 0.971 = 0.029$$

Interpretation: Small gain means this split doesn't help much in creating purer subsets. We should try other splits!

• Weighted entropy generalizes normal entropy.

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- · Always normalize weights before computing probabilities.

Pruning and Overfitting

The Problem: Overfitting in Decision Trees

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- Solution: Pruning to control model complexity

Stop growing tree before it becomes too complex:

Maximum depth: Limit tree depth (e.g., max_depth = 5)

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Advantages: Simple, computationally efficient **Disadvantages**: May stop too early, miss good splits later

Grow full tree, then remove unnecessary branches:

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- **Disadvantages**: More computationally expensive

Systematic approach to find optimal tree size:

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 - 3. At each α , prune branches that increase cost

Systematic approach to find optimal tree size:

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Process:

- 1. Start with full tree ($\alpha = 0$)
- 2. Gradually increase α
- 3. At each α , prune branches that increase cost
- 4. Select α with best cross-validation performance

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- **Domain knowledge**: Consider interpretability requirements

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